BARD Final Report US-4962-16 R

Developing advanced chemical and computational methods for assessing organoleptic properties of olive oil

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Project award year: 2016
Three year research project

Binational Agricultural Research and Development Fund (BARD Fund)

Developing advanced chemical methods for assessing organoleptic properties of Virgin Olive Oil as a tool for improving its quality
Final Report_Abstract (07/01/2016-03/31/2020)

Project objectives

The overall goal of the proposed study is to develop instrumental methodology that will assist the existing human panel to assess organoleptic characteristic of virgin olive oil and to identify the main cause for sensory defects in the oil. To achieve this goal we will meet the following specific objectives;

1. Allocate and produce virgin olive oil which will contain different major sensory defects.
2. Measure chemical parameters such as fatty acid profiles and total phenols of virgin olive oil.
3. Identify and quantify the specific chemical compounds that are related to each defect.
4. Calibrate and validate the electronic nose and electronic tongue methods for detecting sensory defects of virgin olive oil.
5. Establish a database of chemical compounds and sensory properties of virgin olive oil made in Israel and the US and identify the major defects, which will allow us to assess the main causes for the oil deterioration.
6. Create a validated classification tool that will be trained on the analyzed data to predict the quality of olive oil samples.

Background

In Israel, olive is the leading crop among fruit trees in term of planted area with more than 30,000 ha. In the US, the olive oil industry is growing rapidly due to agricultural innovation and consumer demand. However, the world olive oil trade is currently dominated by Spain, Greece and Italy, with many other countries seeking to gain a share. To penetrate the world market and to compete successfully with imported cheap virgin olive oil, Israel and the US have to produce the highest quality olive oil they can. Virgin olive oil quality parameters are defined both by chemical and sensory parameters. While quantification of the chemical parameters is performed objectively through instrument-based methods, the sensory quality evaluation is based only upon human panels. The sensory panel is often subjective, has less repeatability, suffers from fatiguing and requires long and costly training. Therefore it is essential to develop advanced tools to assess the sensory criteria for virgin olive oil aiming to obtain extra virgin olive oil which is the highest grade of olive oil with zero defects and more than zero fruitiness based on the International Olive Council standards. With chemical and computational methods developed from the project, an oil with a sensory defect can be traced back to its flawed fruit or processing step.

Major conclusions, solutions, achievements

A total of 241 olive oil samples, including 191 samples produced with certain sensory defects and 50 commercial samples labeled as “Extra Virgin” from Israel and the US supermarkets, were produced/collected in Israel and the US. Data of 88 parameters of *each* sample were generated from various chemical analyses (i.e. e-tongue, e-nose, quality parameters, total phenol, phenolic profile, fatty acid profile, and volatiles) and sensory analysis. For commercial samples labeled as “Extra Virgin”, 27% from the US and 60% from Israel had sensory defects, respectively. E-tongue data suggested high linear regression coefficients (r^2 = 0.85 for total phenol content) were found between bitterness, pungency and total phenol content of rancid samples to the combined measured values of e-tongue sensors C00 and AE1. E-nose data suggested that more than 70% of the rancid and fusty samples were correctly predicted in their class using discrimination analysis. Machine learning models were then built to predict sensory attributes (positive and negative) using various chemical parameters (e.g. phenolics, volatiles, etc.): outliers were identified using the local outlier factor algorithm; random forest and artificial neural network models were used and the forward feature selection yielded a different number of features for each of the normalized, and non-normalized data.

Implications (scientific and agricultural)

The chemical and computational methods developed in this study help to point out the main causes for olive oil deterioration (as expressed by appearance of sensory defects) and allow adjustment to the production protocols to produce the highest quality oils. The advanced methodology to detect sensory defects in oil will assist the existing sensory panels to allow the industry to test their oils regularly and receive reliable and reproducible feedback at a reasonable price. The sensory defects detected in commercial extra virgin olive oil sold in both countries suggested the importance and urgency of enforceable olive oil standards in both countries. The findings will help the establishment/revision of enforceable olive oil standards and benefit both production and selling of guaranteed high quality olive oil in Israel and the US.

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Final Report_Contribution of the Collaboration (07/01/2016-03/31/2020)

During the funding period, each team brought unique experiences and expertise throughout the project. Detailed contribution from each team is listed below;

1. **Dag Lab (Agricultural Research Organization - Volcani Center, Israel):**
    a. Produced a total of 191 olive oil samples with different sensory defects using a laboratory mill.
    b. Obtained 20 commercial olive oil samples (labeled as "Extra Virgin") from supermarkets in Israel.
    c. Distributed samples to the Benjamin Lab in Israel and the Wang Lab in the US for chemical analyses.
    d. Performed sensory analysis on 211 samples produced/collected in Israel using an International Olive Council certified sensory panel in Israel.

2. **Wang Lab (University of California, Davis, USA):**
    a. Collected 30 commercial olive oil samples (labeled as "Extra Virgin") from the US supermarkets and distributed to the Benjamin Lab and the Dag Lab in Israel.
    b. Conducted all the proposed chemical analyses (e.g. quality parameters, fatty acid profile, total phenol, volatiles, and phenolic profile) except for e-tongue and e-nose analyses on 241 samples in the UC Davis Olive Center chemistry laboratory in the US.
    c. Performed sensory analysis on 30 supermarket olive oil collected in the US using an American Oil Chemists' Society (AOCS) certified sensory panel.
    d. Compiled data from each lab to send to the Tagkopoulos Lab for data analysis.
    e. Communicated with each lab regarding project progress in an effective manner.

3. **Benjamin Lab (Tel Hai College, Israel):**
    a. Performed e-tongue and e-nose analyses on 241 olive oil samples from Israel and the US.
    b. Compared and validated e-tongue and e-nose results with the sensory panel feedback using cross-selective discrimination and multivariate analysis methods to point out sensory defects.

4. **Tagkopoulos Lab (University of California, Davis, USA):**
    a. Calculated the correlation (mutual information, spearman rank coefficient and Pearson correlation coefficient) of various chemical compounds and other major quality parameters to the sensory labels and quality ratings.
    b. Calculated the covariance of all compound pairs that showed differential expression for different sensory defects and sensory panel quality labels, to identify pairs of compounds that have higher chances of co-exist in the samples.
    c. Created an Ensemble classifier tool to predict the olive oil quality, given user-defined chemical markers.

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Final Report_Achievements (07/01/2016-03/31/2020)

Significance of main scientific achievements or innovations

1. Of 50 commercial olive oil samples (30 from the US and 20 from Israel) purchased from supermarkets, 27% (8 out of 30) and 60% (12 out of 20) of commercial samples labeled as "Extra Virgin" did not meet the Extra Virgin grade by containing at least one sensory defect, respectively.
2. The storage study on three cultivars (i.e. Souri, Barnea, and Arbequina) with four replicates for one year indicated that different cultivars had different tolerance for oxidation and rancidity development.
3. Analytical methods such as phenolic profile based on liquid chromatography – diode array detector and volatile profile based on gas chromatography – mass spectroscopy can be used for the detection of sensory defects of virgin olive oil.
4. Calibration of e-nose and e-tongue can detect sensory defects of virgin olive oil using computational statistical analysis (i.e. principle component analysis and discrimination analysis).
5. An Ensemble classier tool for olive oil quality prediction was built by applying various linear and non-linear classifiers including Support Vector Machines, Artificial Neural Networks, Random Forests, Bayesian techniques and Generalized Linear Models on chemical data after first order analysis (i.e. correlation between individual chemical compound and covariance of all compound pairs) and corresponding sensory results from e-tongue, e-nose, and human panel.

Agricultural and/or economic impacts in progress

1. Dissemination of the study results to educate researchers, producers, consumers, and regulatory agencies through local professional journals; scientific literature in peer-reviewed journals; Extension efforts in Israel and the US; and workshops, short courses (e.g. Sensory Evaluation of Olive Oil and Master Milling Certificate Course offered at the

UC Davis Olive Center), and conferences (e.g. “Research in Olive” organized by Dr. Dag in Israel).

2. Recommendation of best practices on fruit storage and oil processing techniques to olive oil producers in Israel and the US to facilitate with increased olive oil yield and improved olive oil quality (with no sensory defects) in upcoming harvest seasons, ensuring a higher premium for olive oil producers.
3. Results of commercial olive oil not meeting the Extra Virgin grade as labeled suggested the importance and urgency of enforceable olive oil standards in both countries. The implementation of such standards will help both countries to penetrate the world olive oil market and to compete successfully with cheap imported virgin olive oil.
4. Development of the computational infrastructure in this study help to create next generation data-driven quantitative tools to easily and effectively detect sensory defects in an olive oil. This tool can be utilized by researchers, producers, and regulatory agencies at an affordable cost.

Publications for Project US-4962-16 R

Status	Type	Authors	Title	Journal	Vol:pg Year	Coun